BATTERY MATERIALS: STRUCTURE AND CHARACTERIZATION

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ABSTRACT

BNL has several research programs related to electric and hybrid vehicles. This includes work on lithium and metal hydride batteries and on direct methanol fuel cells. All of these programs include the synthesis of new materials and the use of the unique facilities at BNL to do *in situ* characterization of electrode materials. In situ characterization involves the use of the facilities at the National Synchrotron Light Source (NSLS) to do both high resolution x-ray diffraction (XRD) and x-ray absorption (XAS) on electrodes in operating cells. The High Flux Beam Reactor is used for neutron scattering studies of metal hydrides. XAS is an ideal method for *in situ* studies of battery materials because both the probe and signal are penetrating x-rays. A major advantage is that XAS is element specific, and this permits investigation of the environment of a constituent element in a composite material. This makes it a very powerful technique for the study of electrode additives and the corrosion of individual components of complex metal hydride alloys. The near edge part of the spectrum (XANES) provides information on oxidation state and site symmetry of the excited atom. This is particularly useful in the study of corrosion and the oxidation changes in cathode materials during the charge/discharge cycle. The extended fine structure (EXAFS) gives structural information. Thus the technique provides both chemical and structural information. Since XAS probes only short range order it can be applied to the study of amorphous electrode materials and electrolytes. In the case of Pt and Pt alloy fuel cell catalysts XAS can be used to measure the occupancy of Pt *d* states, an important parameter in determining electrocatalytic activity.